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    prof., red.; BELOSHAPKO, P.A., prof., red. [deceased]; ZIMAKIN,
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kand.med.nauk; ZHMUR, V.A., prof.; MAKEYEVA, O.V., doktor med.
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PARAY-KOSHITS, M. A.

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PA 3876

USSR/Chemistry - Crystal Structure   Nov 1947
   Chemistry - Nitro Compounds

"Crystalline Structure of Potassium Tetranitropalla-
dite," M. A. Poray-Koshits, Laboratory of Crystallog-
raphy, Institute of General and Inorganic Chemistry
iment N. S. Kurnakov, Academy of Sciences of the USSR
2½ pp

"Dok Ak Nauk" Vol LVIII, No 4

Author undertook the study of the structure of
K₂Pd(NO₂)₄, on recommendation of Prof G. B. Bok, in
connection with the problem of orienting isomers,
which has already been studied. Nitro compounds ap-
pear to be the most favored compounds for conducting

USSR/Chemistry - Crystal Structure (Contd)   Nov 1947   3876

experiments in this field. Briefly describes his ex-
periments and discusses his results. Submitted by
Academician I. I. Chernyaev, 10 Apr 1947.

PORAY-KOSHITS, M.A.

C A

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ASO-ILA METALLURGICAL LITERATURE CLASSIFICATION

PA 60TI1

PORAY-KOSHITS, M. A.

Mar 1948

USSR/Chemistry - Isomers
Chemistry - Films

"In the Department of Chemical Sciences" $3\frac{1}{2}$ PP

"Vest Ak Nauk SSSR" No 3

Dec session held 30-31 Dec 1947. M. A. Poray-Koshits submitted paper, "New Possible Aspects on Isomers in Inorganic Compounds," and A. N. Krotova, "Electrical Nature of Tearing Films From Various Surfaces." Laboratory of Intermediary Products submitted report on the kinetics of some oxidizing actions in mixtures subjected to cooling.

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CA PORAY-KOSHITS, M.A.   6

X-ray investigation of the structure of Gros salt, [Pt-(NH₃)₄Cl₂]Cl₂. G. B. Bokii and M. A. Poral-Koshits. *Izvest. Sektora Platiny i Drugikh Blagorod. Metal., Inst. Obshchei i Neorg. Khim., Akad. Nauk SSSR* No. 24, 52-59 (1949). --The crystal structure as detd. roentgenographically is tetragonal body centered. The lattice consts. are a 7.41 A. and c 7.98 A. There are 2 mols. of [Pt-(NH₃)₄Cl₂]Cl₂ per unit cell. The space group D_{4h}^{17} = $I4/mmm$. Parameters of atoms are, in fractions of axis and in A., resp.: Pt (2) x = y = z = 0, x = y = z = 0; NH₃ (8) x = y = 0.194, z = 0, x = y = 1.44, z = 0; Cl₁ (4) x = y = 0, z = 0.281, x = y = 0, z = 2.95; Cl₁₁ (4) x = 0.5, y = 0, z = 0.25, x = 3.72, y = 0, z = 2.99). Within the complex Pt(NH₃)₄Cl₂ the distances between the atoms are Pt-NH₃ = 2.03, Pt-Cl = 2.25, NH₃-NH₃ = 2.86, and -NH₃-Cl = 3.04 A. The distances between atoms of adjacent complexes are NH₃-Cl = 3.65, Cl-Cl = 3.48 A. The distances between atoms in the complex and ions in the outer sphere are: NH₃-Cl⁻ = 3.36, Cl-Cl⁻ = 3.73 A. The Cl⁻ have a coördination no. of 12; the 8 NH₃ are closer than the 4 Cl. The smallest distance between Cl⁻ in the outer sphere is 3.90 A.   M. Hosch

PORAY-KOSHITS, M.A.

C A

2

Crystal structure of [Pt(NH₃)₄Cl₂]Cl₂. G. B. Bokil and M. A. Poray-Koshits. *Doklady Akad. Nauk S.S.S.R.* 64, 337-9(1949).—The yellow salt described by J. Gros (*Ann. chim. Pharm.* 27, 249(1838)) is uniaxial, $n_\gamma > 1.85$, $n_\beta = a_o = 1.73$. By Debye-Scherrer diagrams, the lattice is tetragonal, space group $D_{4h}^{17} = I, 4/mmm$, $a = 7.41 \pm 0.04$, $c = 7.08 \pm 0.04$ A., $z = 2$. The structure is derived from that of K_2PtCl_6 (Ewing and Pauling, C. A. 23, 2963) through replacement, in each complex, of 4 coplanar Cl atoms by 4 NH₃ groups, and of the outer K⁺ ions by Cl⁻ ions; this gives the *Strukturbericht* type $J_{62} = K_2OsO_2Cl_4$ (*Strukturbericht* 3, 122, 467(1933-35)). The atom coördinates in the elementary cell are, in fractions of the axes (in A. units): Pt(2) $x = y = z = 0$; NH₃(8) $x = y = 0.194$ (1.55), $z = 0$; Cl I (4) $x = y = 0$, $z = 0.281$ (2.25); Cl II (4) $x = 0.5$ (3.72), $y = 0$, $z = 0$. Distances (in A.) within the complex, Pt–NH₃ = (2.00), Pt–Cl = 2.25, NH₃–NH₃ = 2.96, NH₃–Cl = 3.04. Distances between neighboring complexes, NH₃–NH₃ = 4.16, NH₃–NH₃ = 4.54, NH₃–Cl = 3.65, Cl–Cl = 3.48. Distances between atoms of the complex and outer ions, NH₃–Cl⁻ = 3.36, Cl–Cl⁻ = 3.73 A. The coördination no. of Cl⁻ ions is 12, with 8 NH₃ groups nearer than 4 Cl atoms. The least distance between Cl⁻ ions is 3.99 A.   N. Thon

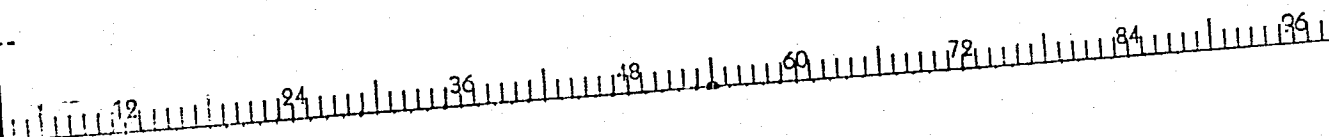PORAY-KOSHITS, M. A.

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PORAY- KOSHITS, M.A.

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Precise determination of the atomic coördinates in the structure of Gerhardt's salt, trans-(NH$_3$)$_2$Cl$_2$Pt. G. B. Bokii, M. A. Poraĭ-Koshits, and G. N. Tishchenko. *Izvest. Akad. Nauk S.S.S.R., Otdel. Khim. Nauk* 1951, 481–6.—Röntgenographic methods were used to study the structure of (NH$_3$)$_2$Cl$_2$Pt. The Pt-NH$_3$ distance is 2.00 A.; the Pt-Cl distance is 2.30 A.   Gladys S. Macy

PORAY-KOSHITS, M.A.

The structure of crystals of the β-modification of rubidium tetrani-
tropalladite.   Trudy Inst.Krist., Akad. Nauk S.S.S.R. 6, 147-54 '51.
(CA 47 no.15:7282 '53)   (MLRA 4:10)

PORAY-KOSHITS, M.A.

Isomorphism of crystals of rubidium and cesium tetranitropalladite.
Trudy Inst. Krist.Akad Nauk S.S.S.R. 6, 155-62 '51.   (MLRA 4:10)
(CA 47 no.15:7282 '53)

PORAI-KOSHITS, M. A.

Structure of crystals of dichlorotrapyridinenickel and dichlorotetrapyridinecobalt. M. A. Porai-Koshits and A. S. Antsishkina. Doklady Akad. Nauk S.S.S.R. 92, 333-5 (1953).—Ni$(C_5H_5N)_4Cl_2$ (I) and Co$(C_5H_5N)_4Cl_2$ (II) belong to the ditetragonally dipyramidal form of symmetry with space group D_{4h}^{20} = 14/acd. The unit cell dimensions are: for I a 15.8 and c 16.9 A.; for II a 15.9 and c 17.0 A. In each unit cell 8 mols. are present. The Cl atoms enter the inner sphere of the complex. The structure of the crystals is based on mol. octahedra of trans-MPy_4Cl_2 type (diagrammatic disposition is given in a figure). The analysis of electron d. shows that all 4 pyridine rings are rotated relative to the plane of the coördination square MN_4 to the same extent: 45° angle. In half of the complexes of a unit cell the py groups are rotated clockwise; in others, counterclockwise. In complexes aligned along the z axis these rotations alternate. By the methods summarized by Booth (C.A. 39, 4536^0) the following distances were calcd.: Ni-Cl 2.387 ± 0.005, Ni-N 2.00 ± 0.05, Co-Cl 2.32 ± 0.01, Co-N 1.99 ± 0.05. These show the covalent nature of the metal link to all 6 addends. The interatomic distances within the pyridine rings are approx. the same as within structures of org. crystals. Distances between proximate C and H atoms of 2 different py groups of the same mol. and atoms of H and Cl of the same mol. are substantially less than the sum of intermol. radii (by 0.35); this indicates considerable repulsion forces within the mol. and possibility of formation of Cl ions in soln. Packing coeff. of the mols. is 0.73.   G. M. K.

PORAY- KOSHITS, M·A·

Structure of crystals of trans-dichlorodiammineplatinum.
M. A. Poraï-Koshits. *Trudy. Inst. Krist., Akad. Nauk S.S.S.R.* 9, 229-38(1954); cf. *C.A.* 48, 3838b.—trans-Dichlorodiammineplatinum (NH_3)$_2Cl_2$Pt belongs to the monoclinic syngony and prismatic class. The axial ratios are: $a:b:c = 1.348:1:0.901$. The ns are: $n_\gamma = 1.851$; $n_\beta = 1.778$; $n_\alpha = 1.706$. The dimensions of the elementary cell are: $a = 8.07$; $b = 6.05$; $c = 5.46$ kX; $\beta = 93°47'$. The space group is: $C_{2h}^5-P_2/a$. An elementary cell contains 2 mols. The coördinates of the atoms are: Cl (0.244, 1.745, 1.495 kX), NH_3 (1.45, −1.073, 1.331 kX). The at. distances are: Pt-Cl = 2.30 kX; Pt-NH_3 = 2.17 kX. The orientation of the complexes of mols. is detd. by the angles that the perpendicular to the plane of the complexes forms with the axes x, y, and z: 35.7°, 63.2°, 65.9°.   E. G. M.

PORAY-KOSHITS, M.A.

Category : USSR/Solid State Physics - Structural Crystallography   E-3

Abs Jour : Ref Zhur - Fizika, No 2, 1957 No 3690

Author   : Poray-Kashits, M.A.
Title   : On the Reduction of the Values of Structural Amplitudes to an
           Absolute Scale

Orig Pub : Tr. In-ta kristallogr, AN SSSR, 1954, 9, 305-312

Abstract : See Ref. Zh. Khim. 1956, 49953

           Inst. Gen. + Inorganic Chem im N.S. Kurnakov, A.S. USSR

Card   : 1/1

PORAY-KOSHITS, M.A.

X-ray structure of complex compounds of bivalent cobalt and nickel. M. A. Poraĭ-Koshits. *Trudy Inst. Krist., Akad. Nauk S.S.S.R.* 10, 117-35(1954).—Cs$_2$CoCl$_4$ has orthorhombic-pyramidal crystals with $a:b:c = 0.755:1:0.568$; biaxial, $\gamma = 1.584$; $\beta = 1.579$; $a = 1.575$; $a_0 = 9.737 \pm 0.005$, $b_0 = 12.972 \pm 0.001$, $c_0 = 7.392 \pm 0.003$ A.; $Z = 4$; space group $D_{2h}^{16}-Pnma$; K$_2$SO$_4$ structure-type, with tetrahedral [CoCl$_4$] units, in agreement with electron-diffraction results of Finsker and Tishchenko. The at. coördinates and interat. distances are tabulated (18 parameters). The tetrahedra are slightly distorted, but not so much as in Cs$_2$[CuCl$_4$] (cf. Helmholz and Kruh, C.A. 46, 6158b). The Co-Cl bond length is const. (2.23 $\pm$ 0.01 A.), of covalent type, but different from that in Cs$_2$CoCl$_4$ (2.34 A.). Four of the 11 Cs$^+$ around [CoCl$_4$] have a distance Cs-Cl = 3.52 A., 5 Cs$^+$ the distance 3.69 A., and two the distance 3.94 A. The structure of Cs$_2$[CoBr$_4$] is analogous, and tetrahedral groups also occur in Cs$_2$CoCl$_4$, (NH$_4$)$_2$[Co(NCS)$_4$].H$_2$O, and K$_2$[Co(NCS)$_4$].H$_2$O. Only in Co phthalocyanine a different coördination type appears caused by the large and rigid org. network in the compd. The conclusions of Cox, *et al.* (C.A. 31, 8416^7) that Co may appear equally well in tetrahedral as in quadratic coördinations are incorrect; only Cu has such a variable coördination character. Ni^{2+} is typically coördinated to quadratic configurations with anions in Ba[Ni(CN)$_4$].4H$_2$O, Sr[Ni(CN)$_4$].5H$_2$O, Na$_2$[Ni(CN)$_4$].3H$_2$O, K$_2$[Ni(C$_2$S$_2$O$_2$)$_2$], Ni dimethylglyoxime, Ni phthalocyanine, while Ni(CO)$_4$ has a tetrahedral configuration, but with the valency of Ni = 0. The distinguishing properties of Co^{2+} and Ni^{2+} are evident in many other complexes; isomorphic relations between both cations are dominant only if [MeX$_4$] coördinations occur. K$_2$CoF$_4$ and K$_2$NiF$_4$ have cubic syngony, but are typically defective structures of the perovskite type which is observed in KNiF$_3$; $^1/_2$ of the octahedral positions are statistically left empty. The crystals show a slight optical anisotropy, and are of tetragonal-tabular habit when crystd. from soln., with $a:c = 1:3$ (cf. Balz, C.A. 48, 18e). CsNiCl$_3$ has a LiI.3H$_2$O type of hexagonal structure; the high polarizability of Cl$^-$, and the low counterpolarization.

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M. A. PORAI-KOSHITS

effects of Cs^+ correspond to a strengthening of the bonds Ni-Cl that are not in agreement with the cubic, but rather with the hexagonal-octahedral coördinations observed. $Ni(NH_3)_4(NCS)_2$ is paramagnetic, orthorhombic, optical character neg.; $\gamma = 1.745$; $\beta = 1.732$; $\alpha = 1.559$; $2V = 82°$; $a_0 = 10.7 \pm 0.05$; $b_0 = 10.2 \pm 0.05$; $c_0 = 7.6 \pm 0.05$ A.; $Z = 4$; space group D_{2h}^{16}-$Pbnm$. The Ni coördination is octahedral, of the form $[Ni(NH_3)_4(CNS)_2]$, in trans-trans-cis configuration, with 2 (CNS) groups bonded to the central Ni^{2+} by a N, and one (CNS) group bonded by a S atom; further, the groups are arranged in chains in the symmetry plane (001) in double layers. Interat. distances are: Ni-S = 2.50 A.; Ni-N$_1$ = 2.15 A.; Ni-N_2 = 2.00 A.; Ni-(NH$_3$)$_1$ = 2.00 A.; Ni-(NH$_3$)$_{11}$ = 2.05 A. The structure is of the mol. type, consisting of 6 complex mols. $Ni(NH_3)_4$-(NCS)$_2$; the polyhedra of the complexes around the Ni^{2+} are polar, with the pos. pole of the dipole in the midst of the base of a pyramid erected above the Ni. The polarity of these complexes is immediately lost in the H_2O soln. of the

salt. $Nipy_2Cl_2$, and $Copy_2Cl_2$ are isomorphous, of ditetragonal-bipyramidal symmetry; the Ni salt shows paramagnetism with $\mu_{eff.} = 3.03$; $\gamma = 1.660$; $\beta = 1.021$; $a_0 = 15.8 \pm 0.05$ A.; $c_0 = 16.0 \pm 0.05$ A. The corresponding data for the Co salt are: $\mu_{eff.} = 4.73$; $a_0 = 16.0 \pm 0.05$ A.; $c_0 = 17.1 \pm 0.05$ A. Space group is D_{4h}^{19}-$I4/acd$. The coördination type is trans-$[Mpy_2Cl_4]$ (octahedral), with the 4 pyridine units in the plane (001); half of the pyridine groups are turned clockwise, half counter-clockwise, alternating along the z-axis. Interat. distances are: Ni-Cl = 2.387 $\pm$ 0.005; Co-Cl = 2.33 $\pm$ 0.01; Ni-N = 2.00 $\pm$ 0.05; Co-N = 1.99 $\pm$ 0.05 kX, all showing the covalent character of bonding. The packing d. is rather high ($k = 0.73$), which explains also the perfect cleavage on (100) and the elongated crystal habit. The paramagnetism speaks for the sp^3d^2 hybridization of the bonding electrons, in analogy with the magnetic properties of $[Ni(biarsine)_2](ClO_4)_2$ and $[Ni(bipyridyl)_3](ClO_4)_2$; only the latter compd. has a sp^3d^2 electron configuration (cf. Burstall and Nyholm, C.A. 47, 2622a) with $\mu_{eff.} = 3.0$.

W. Eitel

PORAY*KOSHITS, M.A.

"Roentgeno structural Studies of Complex Compounds of Bi-valent Cobalt and Nickel." by M.A. Poray-Koshits. pp. 269-287.

SO: Works of the Inst of Crystallography. Issue #10. (Reports submitted at the 3rd International Congress of Crystallography; published by the Acad Sci USSR, Moscow, 1954)

Poray-Koshits. M. A.

USSR/Solid State Physics - Structural Crystallography, E-3

Abst Journal: Referat Zhur - Fizika, No 12, 1956, 34611

Author: Poray-Koshits, M. A.

Institution: None

Title: On the Accuracy of the Determination of the Coordinates of Light Atoms in
        Crystals of Complex Compounds of Platinum with Chlor-Aluminum Series

Original Periodical: Izv. sektora platiny is drugikh blagorodnykh metallov IONKh,
                      AN SSSR, 1954, 28, 183-201

Abstract: See Referat Zhur - Khim, 1956, 24885

PORAY-KOSHITS, M.A.

Increasing the precision of the values for the interatomic distances in the structure of a crystal of the trans-dichloro-tetrammine chloride of quadrivalent platinum. M. A. Poraĭ-Koshits and E. M. Romanova (N. S. Kurnakov Inst. Gen. and Inorg. Chem., Moscow). Izvest. Sektora Platiny i Drug. Blagorod. Metal., Inst. Obshchei i Neorg. Khim., Akad. Nauk S.S.S.R. 28, 282-6(1954).—A precise detn. of the lattice parameters for trans-[(NH₃)₄Cl₂Pt]Cl₂ gave the following values a = 7.438 ± 0.002kX, and c = 7.051 ± 0.003kX. The Pt-Cl distance was detd. more accurately by a calcn. of the distribution of the values of the interat. function along the straight line [001] which passes through the coördinate origin. This distance was equal to 2.32 ± 0.05kX. The Cl-Cl distance for ions on the straight line was 3.30 ± 0.10 kX, which is significantly less than the sum of the ionic radii.   J. Rovtar Leach

PORAY-KOSHITS, M.A.

X-ray diffraction study of *cis-tetrachlorodiaminoplatinate.* G. B. Bokii, G. A. Kukina, and M. A. Poral-Koshits. *Izvest. Sektora Platiny i Drug. Blagorod. Metal., Inst. Obshchei i Neorg. Khim. Akad. Nauk S.S.S.R.* No. 29, 5-18(1955).—The x-ray patterns of light-yellow *cis-*[Pt-(NH$_3$)$_2$Cl$_4$] crystals characterize their structure as prismatic with $a = 6.30 \pm 0.05$, $b = 10.75 \pm 0.05$, $c = 11.20 \pm 0.05$ A., $\beta = 96°57'$, space group $C_{2h}^6 - C2/c$ and $C_s^4 - Cc$, $\gamma = 1.955$, $\beta = 1.870$, and $\alpha = 1.855$. Electrons are scattered by the electrostatic potential fields in the crystal lattice, and the scattering power of an atom depends on $(Z - f_x)$, where Z is the at. no. and f_x the scattering factor for x-rays. Since f_x falls further below Z for lighter atoms than for heavier ones, it follows that lighter atoms are relatively better scatterers of electrons than of x-rays. This method was used to yield maps showing both the electron-d. and the distribution of potential in the unit cell.   A. P. Kotloby

PORAY-KOSHITS, M.A.

CH Structure of nickel and of cobalt dichlorotetrapyridine crystals. M. A. Poral-Koshits and A. S. Antsishkina. *Iscest. Sektora Platiny i Drug. Blagorod. Metal., Inst. Obshchei i Neorg. Khim., Akad. Nauk S.S.S.R.* No. 29, 19–36(1955); cf. *C.A.* 48, 3838b.—The crystals of complex compds. $Nipy_4Cl_2$ and $Copy_4Cl_2$ are isomorphic. They belong to a ditetragonal dipyramidic type of symmetry with a space group D_{4h}^{19}-$I4/acd$. The following crystal consts. were detd.: a_{Ni} = 16.9 ± 0.05, c_{Ni} = 17.0 ± 0.05 A., a_{Co} = 16.0 ± 0.05, c_{Co} = 17.1 ± 0.05 A., N = 8. The Cl atoms in both compds. are within the inner shell of the complex mol. Bond lengths in the mols. are: Ni-Cl = 2.387, Ni-N = 2.00, Co-Cl = 2.32, and Co-N = 1.99 kX. These bond lengths indicate the covalent character of forces binding the central atom with its ligand. The C—C bond lengths are approx. the same as in the structures of org. compds.   A. P. Kotlubr

Poray-Koshits, M. A.

Category : USSR/Solid State Physics - Structural Crystallography   E-3

Abs Jour : Ref Zhur - Fizika, No 2, 1957 No 3685

Author   : Poray-Koshits, M.A.
Title   : Derivation of Working Equations for the Electron Density and Structural
            Amplitude on the Basis of the Symmetry and Anti-Symmetry Property of
            Trigonometric Functions.

Orig Pub : Kristallografiya, 1956, 1, No 1, 27-48

Abstract : Analysis of a derivation of the distribution equations for the electron
           density in various spatial groups for all settings; the derivation is
           based on the symmetry and anti-symmetry properties of trigonometric
           functions. The author finds combinations of trigonometric functions
           with even and odd coefficients h, k, and l, corresponding to individual
           elements of the symmetry. The equations corresponding to a set of
           symmetry elements are obtained from a general equation by simply discard-
           ing the trigonometric terms that contradict the required symmetry. The
           relationship between the Fourier coefficients are used only in the final
           stage, when instead of summing from $-\infty$ to $+\infty$ the summation is from zero
           to ∞. The method considered for finding the equations is applicable

Card   : 1/2
           Inst. Gen. & Inorganic Chem. im N.S. Kurnakov

Category : USSR/Solid State Physics - Structural Crystallography   E-3

Abs Jour : Ref Zhur - Fizika, No 2, 1957 No 3685

only to five out of the 230 spatial groups: C_{2v}^{19}, D_{2h}^{24}, T_h^4, O_h^7, O_h^8.
The method can also be used to derive equations for the structural ampli-
tude of crystals of lower syngonies.

Card   : 2/2

Poray-Koshits, M.A.

Category : USSR/Solid State Physics - Structural Crystallography   E-3

Abs Jour : Ref Zhur - Fizika, No 2, 1957 No 3701

Author   : Poray-Koshits, M.A.
Title   : Use of Calculating Machines in X-ray Structural Computations

Orig Pub : Kristallografiya, 1956, 1, No 2, 248-263

Abstract : Survey. Bibliography, 65 titles

Inst. Gen. + Inorganic Chem im N. S. Kurnakov

Card   : 1/1

PORAY-KOSHITS, M. A.

USSR/Physical Chem. Crystals

B-5

Abs Jour : Referat Zhur - Khimiya, No 7, 1957, 22072

Author   : Poray-Koshits, M. A.
Inst   : Not given
Title   : The structure of Tetrachlorcobaltoatacesium CS_2COCl_4

Orig Pub : Kristallografiya, 1956, 1, No 3, 291-299

Abstract : The compound Cs_2CoCl_4 produces rhombic crystals. The para-
           meters of the lattice are: a 9.737, b 12.972, c 7.392 A, Z =
           4, f. gr. Rpat. The positions of the atoms of Cs, Co and of
           the part of atoms Cl are determined in accordance with Pat-
           terson's projection (001) by means of the method of "super-
           position and minimalization." - The greatest degree of pre-
           cision in determining the coordinates was obtained by the
           method of generalized projections with subsequent use of
           Fourier's three-dimensional differential series. The compu-
           tations of the differential series were made with an electron-
           ic calculating machine. The probable errors calculated ac-
           cording to Crookshank's formula have the following values:
           $\epsilon(x)_{Cs}$ 0.003, $\epsilon(x)_{Co}$ 0.005, $\epsilon(x)_{Cl}$ 0.009 A, $\epsilon(CO - Cl)$,
           0.01A. The structure Cs_2CoCl_4 consists of ions Cs+ and of

Card 1/2   -28-

PORAY-KOSHITS, M.A.

Using the methods of "generalized projections" and "added sections"
in structural analysis of crystals. Trudy Inst.Krist.no.12:31-40
'56.   (MLRA 10:2)

1. Institut obshchey i neorganicheskoy khimii imeni Kurnakova Aka-
demii nauk SSSR.
                (Crystallography)

PORAY-KOSHITS, M.A.

Precision calculation with an electronic calculator of the structure parameters of $Ni(NH_3)_4(NCS)_2$ and of Cs_3CoCl_5 by the Fourier method of differential synthesis. M. A. Poraf-Koshits. *Izvest. Akad. Nauk S.S.S.R., Ser. Fiz.* **20**, 740-50 (1956).—The coördinates of the max. of electronic d. were obtained by the method of differential synthesis (cf. A. D. Booth, *C.A.* **40**, 5616³). The space group of $Ni(NH_3)_4$ $(NCS)_2$ is D_{2h}^{16}-*Pbam*. The central Ni atom is surrounded by 4 max., one of S (distance 2.52 kX), 2 of the N from the NCS group (2.02 and 1.98 kX) and 1 N from 1 NH_3 group (2.02 kX). Thus 1 NCS group serves as bridge between 2 Ni atoms and the remaining 2 NH_3 groups are located above and below the plane to give an octahedral symmetry. The space group of Cs_3CoCl_5 is D_{4h}^{18}-*P4/mnc*. The structural type is K_2SO_4, the interat. Co-Cl distances are 2.26 A.
— S. Pakswer

Inst. Gen. + Inorganic Chem. im N. S. Kurnakov, AS USSR

PORAY-KOSHITS, M. A.M ANTSISHKINA, A. S., DIKAREVA, L. M., and YUKHNOV, E. K.

"The Atomic Crystal Structure of Complex Acido-Amine Nickel Compounds" (Section 6-21) a paper submitted at General Assembly and International Congress of Crystallography, 10-19 Jul 57, Montreal, Canada.

C-3,800,199
Institute of General and Inorganic Chemistry, Academy of Sciences (PORAY-KOSHITS, ATSISHKINA, and DIKAREVA)

Moscow University Chemical Faculty (YUKHNOV)

PORAY - KOSHITS, M.A.

70-2-6/24

AUTHOR: Yukhno, E.K. and Poray-Koshits, M.A.

TITLE: The crystal structure of nickel trans-di-isothiocyan-
          otetrammine   (Stroyeniye kristallov trans-diizorodanot-
          etramminnikelya)

PERIODICAL: "Kristallografiya" (Crystallography), 1957, Vol.2,
             No.2, pp.239-248 (U.S.S.R.)

ABSTRACT: Crystals of $Ni(NH_3)_4(NCS)_2$ are monoclinic with space
           group C2/m and unit cell dimensions $a = 11.46 \pm 0.02$,
           $b = 8.18 \pm 0.02$, $c = 5.68 \pm 0.02$ KX and $\beta = 105°$. The compound
           $d_{obs.} = 1.550$ and $d_{calc.} = 1.568$ giving $Z = 2$. The compound
           is paramagnetic with $\mu = 3.31$ Bohr magnetons. The refractive
           indices of the crystals in white light are $n_\gamma = 1.674$,
           $n_\beta = 1.618$ and $n_\alpha = 1.561$ and when freshly prepared the
           crystals are light blue. Retigraph photographs of the zero
           layer for rotation about c and for six layers for rotation
           about b were taken with Mo radiation and the intensities
           were estimated visually. There were 394 reflections in all,
           71 in the xy projection and 97 in the xz. As the Ni
Card 1/2   atoms are fixed by the centering of the cell the Patterson
           projections gave the structure directly which was refined

70-2-6/24

The crystal structure of nickel trans-di-isothiocyanotetra-ammine. (Cont.)

until very close agreement between observed and calculated structure factors was obtained. The reliability factors for the hk0 and h0l zones were (including observed zeros) 0.214 and 0.242 respectively. Final co-ordinates (x, y, z) were:- Ni (0,0,0); N (0.152, 0, 0.293); C (0.240, 0, 0.462); S (0.358, 0, 0.690); NH_3 (0.083, 0.188, 0.834). The Ni atom is six-co-ordinated octahedrally by four NH_3 groups and two NCS groups the latter opposite each other. The lines SCN-Ni-NCS are almost straight. The distances are Ni-N = 2.07 $\pm$ 0.03, Ni-NH_3 = 2.15 $\pm$ 0.02, N-C = 1.20 $\pm$ 0.05, C-S = 1.61 $\pm$ 0.04 KX. The NH_3 groups do not form a perfect square but lie at 3.08 and 3.00 KX from each other. The molecules lie in close packed layers parallel to the 201 plane. Acknowledgments to V.I. Belova and V.A. Koptsik. There are 16 references, 6 of which are Slavic, 8 figures and 3 tables.

ASSOCIATION: Moscow State University im. M.V. Lomonosova.
Card 2/2   (Moskovskiy Gos. Universitet im. M.V. Lomonosova)
SUBMITTED: December 14, 1956.
AVAILABLE: Library of Congress

AUTHOR: Poray-Koshits, M.A., Yukhno, Ye.K., Antsishkina, A.S. and Dikareva, L.M.

TITLE: The atomic crystals structure of complex acido-amine nickel compounds. (Atomnaya struktura kristallov kompleks-nykh soyedineniy nikelya atsidoaminovogo tipa)

ABSTRACT: The purposes of the investigations were to find the co-ordination number of the nickel atom and determine the position of the acid residuals X in compounds of the NiA_4X_2 type; to determine the general character of the structure of thio-cyanate-amine compounds (ionic salts, double molecular com-pounds, complex compounds), which fall out at different sol-ution concentrations; to establish analogies and differences in interatomic distances from nickel to addendium in different compounds; to find the configuration and orientation of thio-cyanate groups, to determine the inter-atomic distances and the nature of N...C and C...S bonds.

The investigation of the above mentioned compounds belongs, as a compound part, to the systematic study of crystal chem-istry of complex mickel compounds. It is of interest both in point of the theory of complex compounds in general and because

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70-3-8/20

The atomic crystals structure of complex acido-amine nickel compounds. (Cont.)

it may well give an explanation for the peculiar properties of complex nickel compounds in particular.

Crystal $Ni(C_5H_5N)_4X_2$, where $X = Cl$, Br and NCS, are not isomorphous. The results of the investigations of tetragonal crystals $Ni(C_5H_5N)_4Cl_2$ were published earlier.

Crystals of $Ni(C_5H_5N)_4Br_2$ are orthorhombic; space group Pna; $a = 15.8$, $b = 9.3$, $c = 14.2 \pm 0.1$ kX.; $\sigma = 1.67$ g/cm^{-3}; $N = 4$.

Crystals of $Ni(C_5H_5N)_4(NCS)_2$ are monoclinic; the space group $C2/c$ or Cc; $a = 12.3$, $b = 13.2$, $c = 16.2 \pm 0.1$ kX., $\beta = 120°$; $\sigma = 1.4$ g/cm^{-3}; $N = 4$.

In both cases the structure investigation was carried out by means of Patterson projections, 'weighted' (generalised) Patterson projections of the first layer lines, with subsequent calculation of centrosymmetrical projections of electron density.

In both cases residuals Br and NCS are bound directly with nickel atoms and lie in transposition to each other.

Card 2/7   Crystal $Ni(NH_3)_4X_2$, where $X = NO_2$ and NCS, are isomorphous; space group $C2/m$; $N = 2$.

70-3-8/20

The atomic crystals structure of complex acido-amine nickel compounds. (Cont.)

In the first compound $a = 10.77$, $b = 6.85$, $c = 6.12 \pm 0.02$ kX. $\beta = 128°$; $\sigma = 1.72$ g/cm^{-3} ; in the second $a = 11.46$, $b = 8.18$, $c = 5.68 \pm 0.02$ kX., $\beta = 105°$; $\sigma = 1.55$ g/cm^{-3} .

The structural type of crystals was determined from Patterson projections and electron-density projections. A more precise determination of inter-atomic distances was achieved with the help of 'weighted' electron-density projections of the first layer line; in the final stage, electron-density sections were used. In both compounds acid residuals NO_3 and NCS belong to the inner region of the complex. The molecular six-coordinated octahedral arrangement of the addenda seems to be typical of all nickel compounds of the NiA_4X_2 type, in contra-distinction to the similar Pd and Pt compounds, whose structure is $[MA_4]X_2$.

The results of structure investigation of crystals $Ni(NCS)_2 \cdot 3NH_3$ have already been published (M.A. Poray-Koshits, Proc. Inst. Crystallogr. 1954, 10, 117). The molecular complexes $Ni(NH_3)_3 (NCS)_2$ have the shape of tetrahedral pyramids with Ni atoms in the centre of the base.

Trigonal crystals $Ni(NCS)_2 \cdot NH_4NCS \cdot 3NH_3$ possess considerable piezoelectricity; space group P321; $a = 10.2$ $c = 11.13 \pm 0.02$

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The atomic crystals structure of complex acido-amine nickel compounds. (Cont.)

kX.; $= 1.495$ g/cm^{-3}; $N = 3$. The structure is determined with the help of Patterson-function projections and Harker sections at heights 1/3 and 0 parallel to (001) and also by using electron-density projections along the second-order axis. The atoms are surrounded octahedrally by three molecules NH_3 and three groups NCS after the design a-a, b-b, a-b (edge isomer). Complex anions $\left[Ni(NH_3)_3 (NCS)_3\right]$ are arranged according to cubic close packing, in the octahedral interstices of which ions NH_4^+, surrounded by six sulphur atoms, are to be found.

Crystals $Ni(NCS)_2 \cdot 2NH_4NCS \cdot 2NH_3 \cdot H_2O$, which belong to the cubic system, also possess piezoelectricity; space group I23; $a = 13.41 \pm 0.02$ kX., $\sigma = 1.523$ g/cm^3; $N = 6$. Six octahedral complex ions trans-$\left[Ni(NH_3)_2(NCS)_4\right]^{2-}$ are arranged in all the corners of the eight cubes with edges 1/2a, except the points 0, 0, 0 and 1/2, 1/2, 1/2; these two are occupied by water molecules.

Eight cathions NH_4^+ are in the centres of the same cubes and are surrounded octahedrally by sulphur atoms of the thiocyanate group. The remaining four ammonium groups, together with four

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70-3-8/20

The atomic crystals structure of complex acido-amine nickel compounds. (Cont.)

polar water molecules, form two tetrahedra around two water molecules in the corners of the cubes 0, 0, 0 and 1/2, 1/2, 1/2.

Thus, all the thiocyanate-amine nickel compounds that fall out of the solution are complex in structure type and must be described by the following formulae:

$$Ni(NH_3)_4(NCS)_2, \; Ni(NH_3)_3(NCS)_2, \; NH_4[Ni(NH_3)_3(NCS)_3],$$
$$(NH_4)_2[Ni(NH_3)_2(NCS)_4]H_2O$$
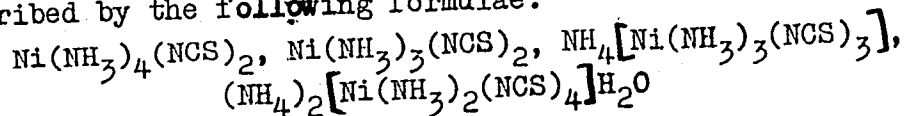
We succeeded in determining all inter-atomic nickel-addendum distances with sufficient precision only in centro-symmetrical structures. The distances are entered in Table 2, p.378, showing that in $Ni(C_5H_5N)_4Cl_2$ and $Ni(NH_3)_3(NCS)_2$ all the nickel-addendum bonds are of covalent character.

The Ni-S distance in the second compound is the contact of different molecules, which completes the nickel co-ordination to six.

The Ni-Br and Ni-NCS distances in bromine- and thiocyanate-pyridine complexes, equal to 2.58 and 2.0 kX., also correspond to covalent bonds.

Card 5/7   In spite of the isomorphism of $Ni(NH_3)_4(NCS)_2$ and

70-3-8/20

The atomic crystals structure of complex acido-amine nickel compounds. (Cont.)

$Ni(NH_3)_4(NO_2)_2$, the relation between inter-atomic metal-addendum distances is quite different. In the first case it is the distances to four neutral substitutes that are increased; in the second, the distances to two acid residuals. Somewhat shortened distances between groups NO_2 and oxygen atoms of neighbouring molecules in $Ni(NH_3)_4(NO_2)_2$ lead us to suppose the existence of weak inter-molecular hydrogen bonds. The abnormal colour of this compound may be accounted for by these structure peculiarities.

All the compounds containing NCS groups are isothiocyanates. In all cases linear groups NCS lie on one straight line with the Ni-N bond direction.

Group dimensions: in $Ni(NH_3)_3(NCS)_2$, $N_I - C_I = 1.15 \pm 0.05$, $C_I - S_I = 1.64 \pm 0.04$, $N_{II} - C_{II} = 1.12 \pm 0.05$, $C_{II} - S_{II} = 1.70 \pm 0.04$ Å kX.; in $Ni(NH_3)_4(NCS)_2$, $N - C = 1.20 \pm 0.05$, $C - S = 1.61 \pm 0.04$ kX.

In spite of the varying distances it is obvious that the N - C bond becomes shorter, and C - S longer, as compared to

Card 6/7

SOV/70-3-6-4/25

AUTHORS: Antsyshkina, A.S. and Poray-Koshits, M.A.

TITLE: X-ray Structural Investigations of the Ni^{II} and Co^{II} Compounds of the type $MePy_4X_2$ (Rentgenostrukturnoye issledovaniye soyedineniy Ni^{II} i Co^{II} tipa $MePy_4X_2$)

Part II. The Structures of Crystals of Dibromotetra-pyridine-nickel and dibromotetrapyridine-cobalt (II. Struktura kristallov dibromotetrapiridin-nikelya i dibromdetrapiridin-kobal'ta)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 6, pp 676-685 (USSR)

ABSTRACT: Crystals of $NiPy_4Br_2$ (green) and $CoPy_4Br_2$ (violet-rose) were found to be isomorphous with space group Pna and cell dimensions a = 15.9, b = 9.4, c = 14.0 and a = 15.9, b = 9.5, c = 14.2 Å respectively in each case $\pm$ 0.1 Å . The observed density of the Ni compound was 1.67 giving Z = 4 . The structure was determined from (001), (010) and (100) Patterson projections, followed by the Patterson sections (001) with w = 1/2 and (211) through (0,0,0). The Fourier projection onto (001) was calculated. The reliability factors were R = 0.24 for hk0 and R = 0.03 for h0ℓ .

Card1/3

X-ray Structural Investigations of the Ni^{II} and Co^{II} Compounds of the type $MePy_4X_2$. Part II. The Structures of Crystals of Dibromotetrapyridine-nickel and dibromotetrapyridine-cobalt

F_o and F_c are given for hk0 projection.

The atomic co-ordinates are shown in a figure on p 679 and in Table 6.

The Ni is six-co-ordinated octahedrally with the Br-atoms in the trans-position. The planes of the pyridine groups are tilted at 45-55° to the plane of the MeN_4 square.

The molecular symmetry is approximately 422.

The magnetic moments were found to be $\mu_{Ni} = 3.03$ and $\mu_{Co} = 4.56$ Bohrmagnetons. Tables of interatomic distances are given. Acknowledgments to A.A.Levin.

Card 2/3

SOV/70-3-6-4/25

X-ray Structural Investigations of the Ni^{II} and Co^{II} Compounds of the type MePy$_4$X$_2$. Part II. The Structures of Crystals of Dibromotetrapyridine-nickel and Dibromotetrapyridine-cobalt

There are 5 figures, 7 tables and 6 references, 4 of which are Soviet and 2 English.

ASSOCIATION: Institut obshchey i neorganicheskoy khimi (Institute of General and Inorganic Chemistry)

SUBMITTED: March 5, 1958

Card 3/3

SOV/70-3-6-5/25

AUTHOR: Poray-Koshits, M.A. and Antsyshkina, A.S.

TITLE: X-ray Structural Investigations of Ni^{II} and Co^{II} Compounds of the Type $Me^{II}Py_4X_2$ (Rentgenostrukturnoye issledovaniye soyedineniy Ni^{II} i Co^{II} tipa $Me^{II}Py_4X_2$) Part III. The Structure of Crystals of Di-isocyano-tetra-pyridine-nickel and Di-isocyano-tetrapyridine-cobalt (III. Struktura kristallov diizorodanotetrapiridin-nikelya i diizorodanotetrapiridin-kobal'ta)

ABSTRACT: Crystals of $Ni(NC_5H_5)_4(NCS)_2$ and $Co(NC_5H_5)_4(NCS)_2$ were found to be isomorphous with space group C2/c (or possibly Cc although no piezo-electric effect could be detected) and cell dimensions a = 12.55, b = 13.0, c = 16.6 Å, β = 119°45' and a = 12.48, b = 12.9, c = 16.5 Å, β = 118°30', respectively. (Measurements were to ± 0.1 Å). Z = 4, d_{Ni} = 1.39 . Both compounds were paramagnetic with moments μ_{eff} = 3.01 Bohr magnetons (Ni) and 4.84 (Co). X-ray reflections were recorded with a retigraph (KFOR). Intensities for the zones (100) (010)

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SOV/70-3-6-5/25

X-ray Structural Investigations of Ni^{II} and Co^{II} Compounds of the Type $Me^{II}Py_4X_2$. Part III. The Structure of Crystals of Di-isocyano-tetrapyridine-nickel and Di-isocyano-tetrapyridine-cobalt

and (001) were estimated visually. Corresponding Patterson projections and packing considerations located the heavy atoms. These were confirmed from the syntheses $P_1(uv)$ and $P_1(uw)$.

$$\left[P_1(uw) = 1/v_o \sum_h \sum_k \left| F\ (hkl) \right|^2 \sin 2\pi hu \cdot \sin 2\pi kv \right] .$$

The lighter atoms were found from appropriate Fourier projections. The final parameters are Ni, $(0,0,0)$; $N_{(NCS)}$, $(0.16, 0.08, 0.02)$; C, $(0.25, 0.09, 0.05)$; S, $(0.40, 0.11, 0.08)$; N_{IPy}, $(0.11, -0.06, 0.135)$; N_{IIPy}, $(-0.04, 0.135, 0.07)$; C_I, $(0.25, -0.16, 0.31)$; C_{II}, $(-0.10, 0.28, 0.15)$. The thiocyanate groups enter the inner co-ordination sphere of the Ni or Co, which is

Card2/4   ocathedrally co-ordinated by the 4 pyridine groups and

SOV/70-3-6-5/25

X-ray Structural Investigations of Ni^{II} and Co^{II} Compounds of the Type $Me^{II}Py_4X_2$. Part III. The Structure of Crystals of Di-isocyano-tetrapyridine-nickel and Di-isocyano-tetrapyridine-cobalt

the 2 isocyanate groups, the latter in the trans- position. The NCS bond is to the Ni or Co through the N_o atoms. The NCS group is linear with $N-C = 1.07 \pm 0.06$ Å and $C-S = 1.74 \pm 0.04$ Å . The Ni-N-CS bond angle is 165°. The $Ni-N_{(NCS)}$ bond is 2.12 Å and the $Ni-N_{Py} = 2.03 + 0.06$ Å . These compounds are similar to others of the NiA_4X_2 class in having this octahedral co-ordination.

There are 6 figures, 2 tables and 43 references, 15 of which are Soviet, 8 German, 2 Scandinavian, 1 Spanish, 1 Italian and 16 English.

Card 3/4

ATOVMYAN

PORAY-KOSHITS, Mikhail Aleksandrovich; TISHCHENKO, G. N.; ATOVMJAN, L. O.

"The Crystal Structures of Co, Ni, Cu, Pt-complex Compounds
of the MeA$_2$X$_2$ type"

a report presented at Symposium of the International Union of
Crystallography   Leningrad, 21-27 May 1959

PORAY-KOSHITS, M. A., Doc of Phys-Math Sci -- (Diss) " X-ray Study in

the Field of Complex Fusion of Double-Valence of Cobalt and Nickel,"

Moscow, 1959, 21 pp (Institute of Crystallography, Acad Sci USSR)

(KL 4-60, 114)

M.A. PURAY - Nish.ts

SOV/62-59-3-36/57

S(0)
AUTHOR: None Given

TITLE: General Meetings of the Department of Chemical Sciences of the Academy of Sciences, USSR on October 23 and November 27-28, 1958 (Obshchiye sobraniya Otdeleniya khimicheskikh nauk Akademii nauk SSSR 23 oktyabrya i 27-28 noyabrya 1958 g.)

PERIODICAL: Izvestiya Akademii nauk SSSR, Otdeleniye khimicheskikh nauk, 1959, Nr 3, pp 564-568 (USSR)

ABSTRACT: This is a report on the General Meetings of the Department of Chemical Sciences, AS USSR. On October 23, 1958 the General Meeting of the Department of Chemical Sciences of the AS USSR took place under the chairmanship of Academician N. N. Semenov. A. V. Novoselova delivered a lecture on the "Investigations in the field of Tellurium Chemistry". She emphasized the fact that the interest in tellurium has considerably increased in the course of the last years because of the valuable semiconductor properties of tellurium and numerous tellurides. In her lecture Novoselova reported on the production of pure tellurium, on the investigations of the behavior of admixtures and on investigations of numerous tellurides. The lecturer was asked numerous questions. M. A. Poray-Koshits, Candidate of Physical and Mathematical Sciences spoke on the "Stereochemistry of Complex Compounds of Bivalent Nickel". On the basis of direct X-ray structural analyses carried out at the Institut obshchey i neorganicheskoy khimii AN SSSR (Institute of General and Inorganic Chemistry, AS USSR) and the MGU it was found that all ammonia thiocyanate compounds of nickel which are separated from the solution at different concentrations represent, according to their structural character, complex six-coordination compounds. The analysis of the crystalline structures makes it possible to set up common crystallochemical rules in the series of ammonia thiocyanate compounds. G. B. Bokiy and S. Z. Roginskiy, Corresponding Members, AS USSR, took part in the discussion. M. G. Gonikberg, Doctor of Chemical Sciences spoke on the "Application of High Pressure in the Investigation of the Transition State and the Mechanism of Reaction". By means of experimental data the lecturer proved that the application of high pressure opens new prospects in this field. S. Z. Roginskiy, B. V. Deryagin, Corresponding Members, AS USSR, M. ... Temkin

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and A. I. Kitaygorodskiy, Doctors of Chemical Sciences took part in the discussion. On the occasion of the general meeting held under the chairmanship of Academician A. P. Vinogradov from November 27 to 28, 1958 M. I. Mikitin, Corresponding Member, AS USSR and G. A. Patrosharatskiy, Candidate of Technical Sciences spoke on the "Properties of Low-substituted Cellulose Nitrates and Their Solutions". The following scientists took part in the discussion: S. N. Danilov, Corresponding Member, O. P. Golova, Doctor of Chemical Sciences, et al. N. V. Semenov, Doctor of Chemical Sciences spoke on the "Specific Sorption of Ions of Organic Substances". The synthesis of weakly swelling ion-exchange resins, which cannot absorb certain ions of organic substances allow the establishment of a new effective method of producing chemically pure streptomycin and penicillin. The lecturer was asked many questions. M. V. Vol'kenshteyn, Doctor of Physical and Mathematical Sciences dealt with the "Problems of Statistical Physics of the Polymer Chains". The lecturer and his collaborators have developed a general statistical method of computing the properties of macromolecules which is based on the application of the rotational isomer model. The following scientists took part in the discussions: V. I. Ivanov, Doctor of Chemical Sciences B. V. Deryagin and V. G. Levich, Corresponding Members, AS USSR. V. N. Tsvetkov, Doctor of Physical and Mathematical Sciences spoke on the "Intermolecular Interaction and the Form of Macromolecules in Solutions". The lecturer demonstrated that the molecular weight of the fraction may be determined by a joint determination of the characteristic viscosity and diffusion. B. V. Deryagin, Corresponding Member, AS USSR, M. V. Vol'kenshteyn, Doctor of Physical and Mathematical Sciences and A. I. Kitaygorodskiy, Doctor of Chemical Sciences took part in the discussion.

Card 2/4

SOV/70-4-1-5/26

AUTHORS: Parpiyev, N. A. and Poray-Koshits, M. A.

TITLE: The Structure of Crystals of Ammonium Tetrachloro-
hydroxonitrosoruthenate (Stroyeniye 'kristallov
tetrakhlorogidroksonitrozo-ruteniata ammoniya)

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 1, pp 30-37 (USSR)

ABSTRACT: The crystal structure of $(NH_4)_2Ru(NO)(OH)Cl_4$ has been
completely determined by X-ray methods. Crystals were
assigned by optical goniometry to the class 2/m. There
was no piezoelectric effect. Photographs with NaCl
standards from a retigraph (KFOR) gave cell dimensions
of a=11.26 $\pm$ 0.02, b=6.76 $\pm$ 0.01, c=15.76 $\pm$ 0.02 A,
$\beta=104°35'$. The cell is primitive with Z=4, and
corresponds to the space group $P2_1/c$. The optical
properties are: 2V=+86°, refractive indices are 1.798,
1.779 and 1.757. Three zones were measured, 152
independent reflexions being collected in the h0ℓ zone,
99 in the 0kℓ and 50 in the hk0. The Ru atoms lie in
general positions which were determined from the three
Patterson projections. Electron density syntheses were
constructed using phases from the Ru positions. These

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The Structure of Crystals of Ammonium Tetrachlorohydroxonitro-soruthenate

SOV/70-4-1-5/26

were refined and tables of final F_{obs} and F_{calc} are given with reliability factors for the h0l, 0kl and hk0 projections of 0.22, 0.23 and 0.24 respectively. The atomic parameters (x,y,z) found were Ru (0.284, 0.156, 0.094); Cl_I (0.406, 0.448, 0.125); Cl_{II} (0.238, 0.177, 0.229); Cl_{III} (0.337, 0.135, -0.043); Cl_{IV} (0.171, -0.135, 0.062); OH (0.141, 0.323, 0.032); N (of NO) (0.415, -0.031, 0.168); O (of NO) (0.508, -0.104, 0.187); $(NH_4^+)_I$ (0.056, 0.406, 0.354); $(NH_4^+)_{II}$ (0.311, 0.844, 0.431). The structure consists of NH_4^+ ions with octahedral Ru(NO)(OH)Cl$_4$" complexes in alternation. Four vertices in a square of the Ru coordination octahedron are occupied by Cl$^-$ ions and the No and OH groups are in the trans-position. The distances in the complex are Ru-Cl, 2.35 + 0.02; Ru-N, 2.04; Ru-O, 2.03; Cl-Cl, 3.33. The Ru radius agrees with that found in other compounds. The structure as a whole is approximately a face-centred

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SOV/70-4-1-5/26

The Structure of Crystals of Ammonium Tetrachlorohydroxonitro-soruthenate

assembly of the complex ions.
Acknowledgments are made to Professor G. B. Bokiy for his advice.
There are 6 figures, 4 tables and 5 references, 2 of which are Soviet, 2 English and 1 international

ASSOCIATION: Moskovskiy gosudarstvennyy universitet imeni
M. V. Lomonosova (Moscow State University imeni
M. V. Lomonosov)

SUBMITTED: July 26, 1958

Card 3/3

SOV/70-4-2-3/36

AUTHORS: Levin, A.A. and Poray-Koshits, M.A.

TITLE: X-ray Structure Calculations on the Universal Computing Machine "Strela" (Rentgenostrukturnyye raschety na universal'noy vychislitel'noy mashine "Strela")

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 2, pp 157-162 (USSR)

ABSTRACT: Programmes for the three principal calculations used in structure analysis (calculations of Fourier and Patterson functions, structure factors and refinements of atomic coordinates) have been written by Shedrin and Ageyeva for the Strela 4 machine of Moscow University for all plane groups, for all monoclinic space groups and for 15 orthorhombic groups. A universal programme for all groups has been written by Brusentsov and a programme for statistical sign determination has been written by Rumanova. These are described briefly. The sign determination programme is of particular interest. It has been compiled for the 65 groups (except

D_{2h}^{24}, T_h^4, O_h^7, O_h^8 in 3 dimensions and Pmm, Pmg, Pgg.

Card1/4   Cmm, P4g, P4m in 2 dimensions) for which

X-ray Structure Calculations on the Universal Computing Machine SOV/70-4-2-3/36
"Strela"

$$F_{hkl} = f(hkl)F_{|h||k||l|}$$

is valid where $f(hkl) = +1$ or -1 depending on the
parity of h, k and l or their linear combinations.
The first part of the programme ensures the obtaining of
chains of "banker" structure amplitudes with definite
sign relations between the members of each group. Each
reflexion can be a member of a chain only when its sign
is determine with sufficient certainty by the other members.
The sign is counted as certain if the difference of the
number of pairs determining one sign and the number of
pairs determining the opposite sign is not less than two.
The chain constructing process lasts till there are no
more reflexions which can be found from any of the chains.
All chains are pointed out, with the sign conditions
between their terms, when signs are arbitrarily allocated
to each. There are two later stages to the programme for
Card2/4   determining the true signs of reflexions in the chains and

X-ray Structure Calculations on the Universal Computing Machine
"Strela"

for finding, by Zachariasen's method, the signs of all reflexions from the signs of the "bankers".
Examples of calculations are given:
1) $SbCl_2(C_6H_5)_3$ with space group $P2_12_12_1$. Signs were calculated for 150 (ho$l$) and (ok$l$) reflexions from the Sb, Cl_I and Cl_{II} positions. $\rho(xz)$ and $\rho(yz)$ were computed. In all the calculations took an hour.
2) One Fourier projection from $PbSb_2S_4$ with 100 reflexions was calculated in 20 min.
3) One Fourier projection (plane group pmg) from $ZnPy_2Cl_2$ with 200 reflexions took 20 min. Calculation of 2 000 signs for $P2_1/c$ and $C2/c$ structures with 25 atoms in the unsymmetric units took an hour each.
A three-dimensional electron density calculation for l-prolyl glycine ($P2_1/m$) with 1 200 reflexions took

Card3/4

X-ray Structure Calculations on the Universal Computing Machine SOV/70-4-2-3/36
"Strela"

        about 10 hours because of the long input and output times.
        There are 9 Soviet references.

ASSOCIATION: Institut obshchey i neorganicheskoy khimii
       (Institute of General and Inorganic Chemistry)

SUBMITTED: November 19, 1958

Card 4/4

SOV/70-4-2-17/36

AUTHORS: Poray-Koshits, M.A. and Tishchenko, G.N.

TITLE: On the Crystal Structures of Cobalt and Copper Dithio-cyanopyridinates (O kristallicheskikh strukturakh dirodanodipiridinatov kobal'ta i medi)

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 2, pp 239-241 (USSR)

ABSTRACT: The compounds $Co(NCS)_2 2Py$ and $Cu(NCS)_2 2Py$ were prepared by breaking down the corresponding tetrapyridinates. Their crystals were acicular with good cleavages into [110] prisms. For the Co compound $n_g > 1.780$; $n_p = 1.700$. No piezoelectricity was detected. The cell dimensions were found to be: Co compound, $a = 9.09 \pm 0.02$ Å; $b = 14.60 \pm 0.03$; $c = 5.66 \pm 0.01$; $\beta = 111°$; $Z = 2$, $d_{obs} = 1.55$, $d_{calc} = 1.58$. Cu compound, $a = 9.17 \pm 0.02$Å; $b = 14.31 \pm 0.03$; $c = 5.65 \pm 0.02$; $\beta = 108°$; $Z = 2$; $d_{obs} = 1.54$, $d_{calc} = 1.59$. The extinctions indicated face centering and the group $C2/m$ was established by

Card1/3

On the Crystal Structures of Cobalt and Copper Dithiocyanopyridinates

SQV/70-4-2-17/36

the structure analysis. Patterson projections were made and, with packing considerations, gave the atomic coordinates: Co $(0,0,0)$; S $(0.264,0,0.599)$; C $(0.202, 0, 0.360)$; N $(0.159, 0, 0.187)$; N_{P_y} $(0,0.145,0)$;

C_I $(0.046, 0.195, 0.175)$; C_{II} $(0.046, 0.294, 0.175)$; C_{III} $(0, 0.345, 0)$. It is proposed to make sections in the (010) and $(20\bar{3})$ planes.

The Co compound belongs to the α-series of CoA_2X_2 -type compounds. Each Co atom is in contact, in the (010) plane, with 2 N atoms and 2 S atoms of the NCS groups. N atoms from the 2 molecules of pyridine make the coordination number of the Co up to 6. The NCS' ions form bridges joining one Co to another. The bond lengths are Co - N_{CS} = 2.10 Å; Co - N_{P_y} = 2.12 Å; Co - S = 2.60 Å.

Intermolecular distances correspond to the sums of the van der Waals radii. The S_{CN} - H_{P_y} distance is about

Card2/3   2.87 Å .

SOV/70-4-2-17/36

On the Crystal Structures of Cobalt and Copper Dithiocyanopyridinates

There are 2 figures and 5 references, 2 of which are
Soviet and 2 German, 1 English.

ASSOCIATION: Moskovskiy gosudarstvennyy universitet im.
M.V. Lomonosova (Moscow State University imeni
M.V. Lomonosov)

SUBMITTED: December 17, 1958

Card 3/3

SOV/70-4-2-18/36

AUTHORS: Gilinskaya, E.A. and Poray-Koshits, M.A.

TITLE: On the Crystal Structure of the Intra-Complex Compound Ni[(C$_2$H$_5$O)$_2$PS$_2$]$_2$ (Preliminary Communication)

O kristallicheskoy strukture vnutrikompleksnogo soyedineniya Ni[(C$_2$H$_5$O$_2$)$_2$PS$_2$]$_2$ (Predvaritel'noye soobshcheniye)

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 2, pp 241-242 (USSR)

ABSTRACT: The new type of compounds of dialkyldithiophosphoric acid with a series of transition elements is more stable than would be theoretically expected. The above compound was taken as an example. Crystals from aqueous solution were dark violet and showed the forms {010}, {110}, {001}. The unit cell was found to have a = 8.85, b = 10.35, c = 10.36 kX, β = 102.5°, Z = 2 with the space group P2$_1$/a . Patterson and Fourier projections onto the xy0 plane were made. Ni atoms are at the centres of inversion. S atoms form a square about the Ni with a Ni-S of 2.2 kX which corresponds to covalent bonds.

Card1/2

On the Crystal Structure of the Intra-complex Compound $Ni\left[(C_2H_5O)_2PS_2\right]_2$ SOV/70-4-2-18/36

Refinements are being carried out. A.I. Busev prepared the material. There are 5 Soviet references.

ASSOCIATION: Moskovskiy gosudarstvennyy universitet imeni M.V. Lomonosova (Moscow State University imeni M.V. Lomonosov)

SUBMITTED: December 17, 1959

Card 2/2

5(2)
AUTHOR: Poray-Koshits, M. A.   SOV/78-4-4-5/44

TITLE: The Coordination Number of Divalent Nickel in
            Paramagnetic Complex Compounds (Koordinatsionnoye
            chislo dvukhvalentnogo nikelya v paramagnitnykh
            kompleksnykh soyedineniyakh)

PERIODICAL: Zhurnal neorganicheskoy khimii, 1959, Vol 4, Nr 4,
            pp 730-740 (USSR)

ABSTRACT: X-ray structure analyses and other physico-chemical
            investigations into the paramagnetic complex compounds
            of divalent nickel with non-cyclic radicals show that
            these structures are octahedral. In most cases the nickel
            in these compounds has a coordination number of 6. The
            author doubts that the inner complex compounds of nickel
            have a tetrahedral structure. The paramagnetic nickel (II)
            compounds are isomorphic to the compounds of cobalt (II),
            which have an analogous composition. Therefore cobalt (II)
            probably exhibits octahedral coordination also in these
            compounds. There are 3 figures and 76 references, 17
            of which are Soviet.
Card 1/2

75982
SOV/70-4-5-4/36

24.7200

AUTHORS: Poray-Koshits, M. A., Dikareva, L. M.

TITLE: Study of the Structure of Nickel Dinitrotetraammine
             Crystals by X-Ray Diffraction Methods

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 5, pp 650-657 (USSR)

ABSTRACT: The artificially grown crystals of $Ni(NH_3)_4(NO_2)_2$ were
             overwhelmingly twins. The monocrystals were platy,
             prismatic with rhombic cross sections, octahedron-shaped,
             or they resembled rhombohedrons. Goniometric measure-
             ments proved, however, identical monoclinic symmetry of
             all of them. The predominant faces were (110) prisms and
             (001) pinacoid. The octahedron-shaped crystals had also
             well developed (20$\bar{1}$) faces. Dovetail twins had (001) as
             the contact plane. The refraction indices are $n_\gamma = 1.660$
             ± 0.003, $n_\beta = 1.598 \pm 0.008$, $n_\alpha = 1.491 \pm 0.003$; the angle
             between the optic axes $2V = 69°20'$. The goniometrically
             determined ratio $a:b:c = 1.54:1:0.89_5$ and $\beta = 116°$. The
             lattice constants were determined according to oscillating-
             crystal photographs and refined by the method of error

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Study of the Structure of Nickel Dinitrotetraammine 75982
Crystals by X-Ray Diffraction Methods   SOV/70-4-5-4/36

elimination by comparison of the reciprocal lattice
photographs with that of NCl. The lattice constants are:
a = 10.77 A, b = 6.85 A, c = 6.14 A, β = 116° and a:b:c
= 1.57:1:0.89. The density is 1.79. There are 2
molecular weights per unit cell. The space group is
C2/m. The crystals are piezoelectric. There are no
extinctions except for (001) centering. The crystal
structure is close to that of Ni(NH3)4(NCS)2. The
b-rotation reciprocal lattice levels reveal, besides the
2-fold rotor, 2 pseudosymmetry axes, making the pattern
look like that of an orthorhombic crystal. The pseudo·
symmetry axes are parallel to /001/* and /401/*. They
are believed to indicate the orthorhombic symmetry of
the atomic distribution within ac planes which shifted
by the b-translation generate the monoclinic three-
dimensional lattice. The atomic coordinates determined
according to the Patterson projections and the reciprocal
lattice data point to the composition of the Ni(NH3)4(NO2)2
crystals of slightly stretched octahedra having Ni at
body-centers, NH3 at 4 vertices forming a square, and
NO2 at the remaining 2 vertices. Ni atoms contact only

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Study of the Structure of Nickel Dinitrotetraammine   75982
Crystals by X-Ray Diffraction Methods   SOV/70-4-5-4/36

N atoms but not O or H atoms. The Ni-to-NH3, Ni-to-N,
NH3-to-NH3, and NH3-to-N (of NO2) distances are 2.07,
2.23, 2.95, and 3.05 A, respectively. The elongation
of the O2N-Ni-NO2 axis weakens this bond relative to
Ni-to-NH3 bond, and perhaps produces the anomalous color
of the compound and its unusually large magnetic moment.
There are 3 figures; 5 tables; and 13 references, 7
Soviet, 2 Japanese, 1 U.S., 1 British, 1 Italian, 1
French. The U.S. and British references are: Bailar,
J. C., The Chemistry of the Coordination Compounds,
1956; and Hulme, R., Acta Crystallogr., 5, 144, 1952.

ASSOCIATION: Institute of General and Inorganic Chemistry (Institut
              obshchey i neorganicheskoy khimii)

SUBMITTED: March 17, 1959

Card 3/3

0.0000

76012
SOV/70-4-5-34/36

AUTHORS: Belov, N. V., Vaynshteyn, B. K., Kitaygorodskiy, A. I., Poray-Koshits, M. A., Semiletov, S. A., Shef'tal', N. N.

TITLE: International Fedorov Session on Crystallography Held in Leningrad

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 5, pp 796-800 (USSR)

ABSTRACT: The International Union of Crystallography (IUC) and the Academy of Sciences of the USSR convened an International Session (interim) on Crystallography commemorating the 40th anniversary of the death of the great Russian crystallographer Ye. S. Fedorov. The session, attended by 600 scientists from the USSR, U.K., France, U.S., Japan, Germany, Czechoslovakia, Netherlands, Canada, Australia, and other countries, was held in Leningrad from May 21 to 27, 1959. The major reports were presented to the plenary sessions and some 100 reports to 2 panels. The subject of the 1st panel was crystal-chemical analysis and that of the 2nd panel electron was diffraction studies.

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International Fedorov Session on
Crystallography Held in Leningrad

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The reports to the plenary sessions were presented by the
following Soviet scientists: N. V. Belov (VP of IUC),
V. I. Simonov, V. A. Frank-Kamenetskiy, G. B. Bokiy,
M. A. Poray-Koshits, L. O. Atovmyan, G. N. Tishchenko,
A. B. Ablov, T. I. Malinovskiy, Ye. A. Shugam, V. M.
Levina, Yu. S. Terminasov, Sh. Kh. Yar-Mukhamedov, Ya.
S. Umanskiy, V.I. Iveronova, L. S. Palatnik,V.A. Finkel',
Ye. I Gladyshevskiy, Z. G. Pinsker, G. S. Zhdanov, A. S.
Sonin, I. S. Zheludev, I. G. Ismailzade, I. S. Rez,
A. V. Stepanov, I. B. Borovskiy, A. S. Povarennykh,
Z. V. Zvonkova, A. I. Kitaygorodskiy, O. V. Stavrovskiy,
N. N. Sandakova, N. M. Bashkirov, B. K. Vaynshteyn, I. M.
Rumanova, V. L. Indenbom, I. I. Shafranovskiy, N. P.
Trifonov, B. M. Shchedrin, D. M. Kheyker, M. M. Uman-
skiy, A. V. Shubnikov, V. F. Parvov, and V. V. Semenov.
The reports of the U.S. crystallographers were presented
by R. Pepinsky, D. Harker, W. H. Zachariasen, R. Randle,
J. Donohue, G. Donnay, J. H. D. Donnay, and W. Parrish.
Six reports were presented by British crystallographers,
Card 2/3   2 by German, 2 by Czech, 2 by Dutch and 1 each by

International Fedorov Session on   76012
Crystallography Held in Leningrad   SOV/70-4-5-34/36

French, Canadian, and Japanese crystallographers. The
session admitted five new member nations into IUC, con-
firmed its newly appointed officers, including the
editor of "Acta Crystallographica," A. J. C. Wilson,
appointed G. B. Bokiy as head of the subcommittee for
abstracting the Soviet publications in crystallography,
planned Japan to be the site of the next interim, and
Italy or Israel of the next congress, and solved some
other business matters.

SUBMITTED: July 1, 1959

Card 3/3

5(3)

AUTHORS: Dyatkina, M. Ye., Poray-Koshits, M. A.   SOV/20-125-5-21/61

TITLE: A New Possible Type of Isomerism in the Octahedral
                Complexes of Some Transition Elements, Especially Cu
                (O novom vozmozhnom tipe izomerii v oktaedricheskikh
                kompleksakh nekotorykh perekhodnykh elementov, v
                chastnosti Cu)

ABSTRACT: A cis-trans-isomerism is known to be possible in the
                complexes mentioned in the title, which contain at least
                two kinds of ligands. In the case of a "regular" octahedral
                structure only the aforementioned type of isomerism is to
                be expected except optical isomerism. However, the authors
                try to prove that in several cases additional types of
                isomerism of the aforesaid complexes may occur. According
                to modern conceptions concerning the field theory of
                ligands, distortions are bound to occur under certain
                circumstances in consequence of the Yan-Teller effect. This
                is really the case. This distortion is bound to occur along
Card 1/4   one of the oscillation coordinates. Recently several

A New Possible Type of Isomerism in the Octahedral   SOV/20-125-5-21/61
Complexes of Some Transition Elements, Especially Cu

research workers used these assumptions for the explanation
of the distortion of the regular octahedral arrangement
of ligands around the central atom in the case of the
compounds of Cu (II), Cr (II), and Mn (III) (Refs 1, 2).
It has, however, hitherto been neglected that in the
presence of two types of ligands such distortions may
cause further types of spatial isomerism. In the case of a
tertragonal distortion the existence of two types is in
principle possible: a) one corresponds to an extended
octahedron, b) the other one to a compressed octahedron.
In principle such an isomerism may occur as well in the case
of six equal ligands. However, only distortions of the
type a) have hitherto been found to occur in the case of
equal ligands. An attempt was made (Ref 3) to explain this
fact theoretically. The number of possible isomers in the
case of the composition $AX_2Y_2Z_2$ (see Scheme) is assumed to

be the greatest. In the case of the type of distortion a)
and b) three isomers are possible for each. This depends

Card 2/4   on the fact which of the three couples of ligands lies on

A New Possible Type of Isomerism in the Octahedral   SOV/20-125-5-21/61
Complexes of Some Transition Elements, Especially Cu

the axis which differs from the other ones. The authors
assume that this very type of isomerism holds for the cases
(Ref 4) of $Cu(NH_3)_2Br_2$ and $Cu(NH_3)_2Cl_2$ with a coordination
polyhedron $Cu(NH_3)_2X_4$. It was assumed (Ref 1) that those
ligands that create a less intense field are bound to lie
on the long axes. According to the increasing field strength,
the ligands form a series $Br < Cl < H_2O < C_6H_5N < NH_3 < CH_2NH_2CH_2NH_2$
(Ref 6) so that water and especially ammonia have to tend
towards a position on a short axis, compared with bromine.
This agrees with the structure of the a-isomer and explains
why no b-isomer is produced. In the latter the ammonia
molecules would lie on the longer axis, contrary to the
greater strength of the field produced by them. The
probability of the formation of a compressed isomer b
increases with increasing difference of the field strength
which is produced by various ligands. The above-mentioned
data indicate that the isomerism of Cu (II) compounds

Card 3/4   detected by Hanic (Ref 4) is not only based upon the

A New Possible Type of Isomerism in the Octahedral   SOV/20-125-5-21/61
Complexes of Some Transition Elements, Especially Cu

difference between the quadratic dsp^2-(or sp^2d)-hybridization
and the linear sp-hybridization. The authors assume that all
six ligands lie in all cases in the "internal sphere"
around the copper atom. The existence of isomerism is due
to the distortion of the coordination octahedron in consequence
of the Yan-Teller effect. There are 1 figure and 6 references,
1 of which is Soviet.

ASSOCIATION: Institut obshchey i neorganicheskoy khimii im. Kurnakova
               Akademii nauk SSSR (Institute of General and Inorganic
               Chemistry imeni Kurnakov of the Academy of Sciences USSR)

PRESENTED: December 27, 1958, by I. I. Chernyayev, Academician

SUBMITTED: December 27, 1958

Card 4/4

PORAY-KOSHITS, M. A., BOKIY, G. B.

"5-X-1. The Crystal Chemistry of Complex Compounds of Metals of Group VIII."

Acad. of Sciences, USSR.

paper submitted for 5th Gen. Assembly, Symposium on Lattice Defects, Intl. Union of
Crystallography, Cambridge U.K. Aug 1960.

PHASE I BOOK EXPLOITATION   SOV/4306

Poray-Koshits, Mikhail Aleksandrovich

Prakticheskiy kurs rentgenostrukturnogo analiza, t. II (Practical Course in X-Ray Analysis, Vol. 2) [Moscow] Izd-vo Mosk. univ., 1960. 631 p. Errata slip inserted. 7,000 copies printed.

Eds.: G.B. Bokiy, Corresponding Member, Academy of Sciences USSR, and S.F. Kondrashkova; Tech. Ed.: M.S. Yermakov.

PURPOSE: This book is intended for chemistry and geology students studying structural X-ray analysis.

COVERAGE: The book, Volume 2 of a multivolume work, has been authorized as a textbook for state universities by the Ministerstvo vysshego i srednego spetsial'nogo obrazovaniya SSSR [Ministry of Higher and Secondary Special Education of the USSR]. The book presents a systematic and detailed treatment of modern methods of analyzing the atomic structure of crystals based on the analysis of the diffraction spectrum intensity. This volume consists of Parts IV and V. Part IV treats the theory of the intensity of X-ray diffraction in a crystal and related problems in the preliminary processing of experimental X-ray data. Part V discusses basic methods and practical examples in the determination of

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PORAY-KOSHITS, M.A.

Coordination of Ni atoms in the crystal structure of $Ni(CH)_2NH_3$ nH_2O. Zhur. strukt. khim. 1 no.1:125-126 My-Je '60.

(MIRA 13:8)

1. Institut obshchey i neorganicheskoy khimii imeni N.S.Kurnakova AN SSSR.

(Nickel compounds) (Coordination compounds)

POLYNOVA, T.N.; PORAY-KOSHITS, M.A.

 Crystal structure of triphenyldichlorostibine. Zhur. struk.
 khim. 1 no.2:159-161 Jl-Ag '60. (MIRA 13:9)

 1. Moskovskiy gosudarstvennyy universtite im. M.V. Lomonosova.
     (Stibine)

PORAY-KOSHITS, M.A.; ATOVMYAN, L.O.; TISHCHENKO, G.N.

Crystal structure of isomorphic cobalt and zinc dihalodipyridinates.
(concerning the nature of the isomerism of cobalt compounds having
the composition CoA_2X_2). Zhur. strukt. khim. 1 no.3:337-341 S-O
'60.   (MIRA 14:1)

1. Institut obshchey i neorganicheskoy khimii imeni N.S. Kurnakova
AN SSSR.
            (Cobalt compounds)   (Zinc compounds)

24.7100

78112
SOV/70-5-1-21/3?

AUTHORS: Bukovska, M., Poray-Koshits, M. A.

TITLE: The Crystal Structure of Millon and Becton Salts (Brief
               Communications)

/PERIODICAL: Kristallografiya, 1960, Vol 5, Nr 1, pp 137-140 (USSR)

ABSTRACT: The isostructural $Cu(NH_3)_4 \cdot PtCl_4$ and $Pt(NH_3)_4 \cdot CuCl_4$ were

               produced as violet and green powders, the former also in
               monocrystals. Both are tetragonal, nonpiezoelectric as
               determined by V. A. Koptsik, optically negative with
               n_α = 1.766, n_γ = 1.717, and n_α = 1.879, n_γ =
               = 1.793, respectively, as determined by Ye. V. Pachkin.
               According to the powder and single crystal diffraction
               patterns, the lattice constants of the first compound
               are: a = 9.06 + 0.02 A, c = 6.43 + 0.02 A, density 3.00,
               two molecular weights per unit cell, space group P 4/mnc,
               the atomic positions as shown in Fig. 3. The atomic
               coordinates of Cl are: x = 0.254 A, y = 0.056 A, z =
               0; of NH_3 are: x = 0.217 A, y = -0.059 A, z =

Card 1/3   0.5 A; the accuracies are: +0.01 A for x_{Cl} and +0.03 A

               for x_N. The bond lengths are: Cu-to-NH_3, 2.04 A;

The Crystal Structure of Millon and Becton Salts 78112
(Brief Communications)   SOV/70-5-1-21/30

         Pt-to-Cl, 2.36 A; Cu-to-Pt, 3.21 ± 0.01 A; Cl-to-N,
3.45 ± 0.05 A. Both compounds are isomorph with
$Pt(NH_3^-)_4 \cdot PtCl_4$, but differ slightly with respect to the
bond lengths. There are 3 figures; 1 table; and 6
references, 3 Soviet, 1 German, 1 French, 1 U.S.
The U.S. reference is: M. Atoji, J. W. Richardson,
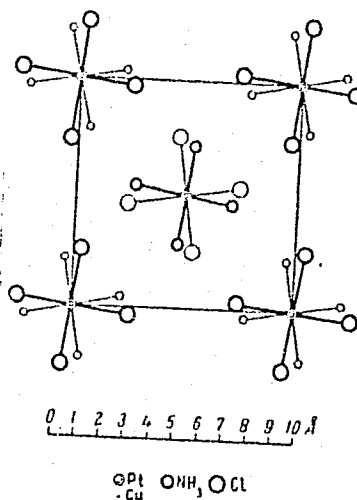R. E. Rundle, J. Amer. Chem. Soc., 12, 3017, 1957.

ASSOCIATION: Moscow State University imeni M. V. Lomonosov (Moskov-
skiy gosudarstvennyy universitet imeni M. V. Lomono-
sova)

SUBMITTED: July 24, 1959

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(Brief Communications)

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$$0 \; 1 \; 2 \; 3 \; 4 \; 5 \; 6 \; 7 \; 8 \; 9 \; 10 \, \text{Å}$$

$\circ$Pt O NH$_3$ O Cl
$\cdot$ Cu

Card 3/3   Fig. 3. Schematic representation of structure of
$[Cu(NH_3)_4] [PtCl_4]$.

24.7100

78113
SOV/70-5-1-22/30

AUTHORS: Bukovska, M., Poray-Koshits, M. A.

TITLE: The Crystal Structure of the Double Salt, Copper
             Perchlorate Pentammine-Ammonium Perchlorate
             (Brief Communications)

PERIODICAL: Kristallografija, Vol. 5, No.1, 140-141, Ja.-F '60.

$Cu(NH_3)_5(ClO_4)_2 \cdot NH_4ClO_4$ crystals, grown from an
aqueous solution of copper nitrate, ammonium
perchlorate, and ammonia, assayed 13.7% Cu, 21.92%
NH_3, 62.35% ClO_4. The tetragonal prismatic blue
crystals were paramagnetic with $\mu = 1.77$ MB, as
determined by N. V. Belova, and piezoelectric, as
determined by V. A. Koptsik. The lattice constants
are a = 10.59 + 0.02 A; c = 7.50 + 0.02 A; measured
density 1.84, calculated density 1.835; 2 molecular
weights per unit cell; space group P $\overline{4}2_1$m. The
atomic coordinates and interatomic spaces are
compiled in Tables 1 and 2, respectively. According

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The Crystal Structure of the Double
Salt, Copper Perchlorate Pentammine-
Ammonium Perchlorate (Brief Communica-
tions)

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SOV/70-5-1-22/30

to the disposition of atoms the formula should be
written as $NH_4 \left[Cu(NH_3)_4 \right] (ClO_4)_3 \cdot NH_3$. There
are 2 tables; and 4 Soviet references.

ASSOCIATION: Moscow State University imeni M. V. Lomonosov
(Moskovskiy gosudarstvennyy universitet imeni
M. V. Lomonosova)

SUBMITTED: July 24, 1959

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CHZHOU KO-SYAN [Chou K'uo-hsiang]; Poray-Koshits, M.A.

Crystal structure of the double salt mercury thiocyanate - nickel thiocyanate hydrate. Kristallografiia 5 no.3:462-463 My-Je '60.
(MIRA 13:8)

1. Moskovskiy gosudarstvennyy universitet im. M.V. Lomonosova.
(Mercury compounds)   (Nickel compounds)

BOKIY, G.B.; PORAY-KOSHITS, M.A.

Crystallography of complex compounds of metals of group 8. Kristal-
lografiia 5 no.4:605-619 Jl-Ag '60.   (MIRA 13:9)

1. Institut obshchey i neorganicheskoy khimii im. N.S. Kurnakova.
                    (Complex compounds)

S/020/60/134/005/015/023
B016/B054

AUTHOR: Poray-Koshits, M. A.

TITLE: Crystal-chemical Data Concerning the Stereochemistry of
              Complex Compounds of Some Bivalent Transition Metals (Fe, Co,
              Ni, Cu, Pd, and Pt)

PERIODICAL: Doklady Akademii nauk SSSR, 1960, Vol. 134, No. 5,
              pp. 1104-1107

TEXT: On the basis of the results of more than 30 X-ray structural
investigations of the complex compounds of the bivalent metals: Co, Ni,
Pd, and Pt, the author finds some characteristic features of the stereo-
chemistry of complex compounds of metals in the horizontal series
Fe, Co, Ni, Cu, and in the vertical series Ni, Pd, Pt. Table 1 gives
statistical data on the coordination polyhedrons of the Fe-, Co-, Ni-,
Cu-, Pd-, and Pt-atoms on the basis of available structural data. Table
2 contains data on the changes in the coordination and the magnetic
state with varying addends in the series CN, NO_2, NCS, Br, Cl, F, O; this
series corresponds to the gradual rise in polarity of the bond, also in

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Crystal-chemical Data Concerning the Stereo-   S/020/60/134/005/015/023
chemistry of Complex Compounds of Some   B016/B054
Bivalent Transition Metals (Fe, Co, Ni, Cu,
Pd, and Pt)

the case of a replacement of an acid addend by a neutral substituent.
1) The compounds of bivalent Pd and Pt are always diamagnetic. Their
complexes have a planar structure, independent of their composition, with
some exceptions. 2) In contrast to Pt and Pd, Ni forms diamagnetic com-
pounds with quadratic configuration of the complexes only with addends
which form covalent bonds in the most intensive manner. Among inner-
complex compounds, the planar coordination is much more frequent. The
other complex compounds of Ni are, as a rule, paramagnetic, and have an
octahedral coordination (with some exceptions). 3) The stereochemistry of
Co^{II} compounds differs considerably from Ni^{II}. In the series of acido
complexes, the transition from low-spin to high-spin compounds occurs much
later, after the NO_2 groups; no planar, but an octahedral coordination M
is characteristic of the low-spin compounds, whereas no octahedral but a
tetrahedral coordination is characteristic of the high-spin compounds -
in the case of NCS, Br, and Cl. Only in the transition to the most
electronegative addends, Fe and O, the coordinations of both Co^{II} and Ni^{II}

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PORAY-KOSHITS, M.A.; ZOKIY, P.M.

Similarity and differences in the structures of crystals of inner-complex copper and zinc compounds. Zhur. strukt. khim. 2 no. 1:20-26 Ja-F '61.   (MIRA 14:2)

1. Moskovskiy gosudarstvennyy universitet im. M.V. Lomonosova.
        (Copper compounds)   (Zinc compounds)

PORAY-KOSHITS, M.A.; BOKIY, G.B.; KUKINA, G.A.

Distorted octahedral complexes of bivalent platinum, palladium, and nickel. Zhur.strukt.khim. 2 no.3:327-329 My-Je '61.

(MIRA 15:1)

1. Institut obshchey i neorganicheskoy khimii imeni N.S.Kurnakova AN SSSR i Institut neorganicheskoy khimii Sibirskogo otdeleniya AN SSSR.

(Platinum compounds) (Palladium compounds) (Nickel compounds)
(Crystallography)

TISHCHENKO, G.N.; ZORKIY, P.M.; PORAY-KOSHITS, M.A.

    Electron diffraction study of the crystal structure of nickel
    and copper inner complex compounds of salicylalimine and its
    derivatives. Zhur.strukt.khim. 2 no.4:434-444 Jl-Ag '61.
                               (MIRA 14:9)
1. Moskovskiy gosudarstvennyy universitet imeni M.V. Lomonosova.
         (Nickel compounds)   (Copper compounds)
               (Salicylaldehide)

POLYNOVA, T.N.; PORAY-KOSHITS, M.A.

Crystalline structure of antimony diphenyl trichloride. Zhur.
strukt.khim. 2 no.4:477-478 Jl-Ag '61.   (MIRA 14:9)

1. Moskovskiy gosudarstvennyy universitet imeni M.V. Lomonosova.
(Antimony compounds)

PORAY-KOSHITS, M.A.

      Structural aspects of nickel and copper dialkylglyoximates.
      Zhur.strukt.khim. 2 no.5:619 S-O '61.   (MIRA 14:11)

      1. Institut obshchey i neorganicheskoy khimii imeni N.S.
      Kurnakova AN SSSR.
                     (Nickel compounds) (Copper compounds)

PORAY-KOSHITS, M.A.; ZORKIY, P.M.

Reply to the letter to the editor by E.A. Shugam and L.M.
Shkol'nikova. Zhur.strukt.khim. 2 no.5:620-621 S-O '61.
(MIRA 14:11)
1. Moskovskiy gosudarstvennyy universitet imeni M.V.
Lomonosova.

(Nickel compounds)   (Copper compounds)
(Shugam, E.A.)   (Shkol'nikova, L.M.)

PORAY-KOSHITS, M.A.; BUKOVSKA, M.

    Structure of crystals of trans-dinitrotetrammine copper.
    Kristallografiia 6 no.3:381-388 My-Je '61.   (MIRA 14:8)

  1. Moskovskiy gosudarstvonnyy universitet imeni M.V. Lomonosova.
    (Amines)   (Copper compounds) (Crystallography)

ZORKIY, P.M.; PORAY-KORSHTS, M.A.

Structure of molecular crystals. Part 1: Graphic determination
of the maximum density distribution of figures on a plane.
Kristallografiia 6 no.5:655-661 S-O '61.   (MIRA 14:10)

1. Moskovskiy gosudarstvennyy universitet imeni Lomonosova.
                    (Crystallography)

ZORKIY, P.M.; PORAY-KORSHITS, M.A.

Calculating the structure of layers in nickel dimethylglyoximate
crystals under the theory of close packing of molecules. Dokl.AN
SSSR 138 no.2:355-357 My '61.   (MIRA 14:5)

1. Moskovskiy gosudarstvennyy universitet im. M.V.Lomonosova.
Predstavleno akademikom N.V.Belovym.
    (Molecular theory)   (Glyoxime)   (Nickel compounds)